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**On**

# SOFTWARE FOR MODELING BIOCHEMICAL REACTIONS

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# Software for Modeling Biochemical Reactions

Cellerator is a computer program that automatically generates and solves differential equations for complex sets of chemical reactions like those in living cells. Cellerator provides a mathematical and computational infrastructure for characterizing reaction pathways and the interactions between complex molecules (e.g., proteins and nucleic acids) and cellular environments. The user effectively defines the pathways by specifying an input set of chemical reactions. Examples include enzymatic reactions, creation and degradation of various chemical species, binding and unbinding reactions, phosphorylation reactions, and transcription and translation of nucleic acids. More complex signals, such as a chemical cascade, can also be specified. Cellerator translates the specifications of chemical reactions into the corresponding set of differential equations, then solves these equations numerically. Cellerator provides an explicit description of output at several steps through the model-generation process; this feature affords flexibility by facilitating intervention by the user to modify the computational model "on the go," as might be desirable, for example, to correct errors.

*This program was written by Bruce Shapiro, Eric Mjolsness, and Andre Levchenko of Caltech for* **NASA's Jet Propulsion Laboratory**.

*This software is available for commercial licensing. Please contact Don Hart of the California Institute of Technology at (818) 393-3425. Refer to NPO-21122.*

## ABSTRACT

The ultimate fate of all living cells is regulated by a complex set of interactions between various proteins and nucleic acids. Some proteins act directly as transcription factors that control the expression of one or more genes. Others interact with one another along a diverse sequence of pathways that eventually act to either increase or decrease the transcription of specific genes. Cellerator provides a new mathematical and computational infrastructure to characterize these pathways and the interactions between these complex molecules and the cellular environment. Pathways are defined by the user in terms of a set of chemical reaction. Examples include enzymatic reactions, creation and degradation of various chemical species, binding and unbinding reactions, phosphorylation reactions, and transcription of and translation of nucleic acids. More complex signals, such as a chemical cascade, can also be specified. Cellerator then translates these equations into the appropriate set of differential equations that are then solved numerically.

## *PUBLICATION

Bruce Shapiro, Andre Levchenko, and Eric Mjolsness, “Automatic Model Generation for Signal Transduction with Applications to Map Kinase Pathways,” International Conference on Systems Biology (ICSB), Tokyo, Japan, November 14-16, 2000.

*Please obtain publications from sources listed.

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